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APPLICATION NO.	FILING DATE	FIRST NAMED INVENTOR	ATTORNEY DOCKET NO.	CONFIRMATION NO.
10/077,036	02/15/2002	Michael Andrew Parker	SJO919990205US1	1965

22865   7590   05/27/2003

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EXAMINER
JOHNSTON, PHILLIP A

ART UNIT	PAPER NUMBER
2881	

DATE MAILED: 05/27/2003

Please find below and/or attached an Office communication concerning this application or proceeding.

-- *The MAILING DATE of this communication appears on the cover sheet with the correspondence address* --

Period for Reply

A SHORTENED STATUTORY PERIOD FOR REPLY IS SET TO EXPIRE **3** MONTH(S) FROM THE MAILING DATE OF THIS COMMUNICATION.
- Extensions of time may be available under the provisions of 37 CFR 1.136(a). In no event, however, may a reply be timely filed after SIX (6) MONTHS from the mailing date of this communication.
- If the period for reply specified above is less than thirty (30) days, a reply within the statutory minimum of thirty (30) days will be considered timely.
- If NO period for reply is specified above, the maximum statutory period will apply and will expire SIX (6) MONTHS from the mailing date of this communication.
- Failure to reply within the set or extended period for reply will, by statute, cause the application to become ABANDONED (35 U.S.C. § 133).
- Any reply received by the Office later than three months after the mailing date of this communication, even if timely filed, may reduce any earned patent term adjustment. See 37 CFR 1.704(b).

Status

1)☐ Responsive to communication(s) filed on _____ .

2a)☐ This action is **FINAL**.   2b)☒ This action is non-final.

3)☐ Since this application is in condition for allowance except for formal matters, prosecution as to the merits is closed in accordance with the practice under *Ex parte Quayle*, 1935 C.D. 11, 453 O.G. 213.

Disposition of Claims

4)☒ Claim(s) *1-69* is/are pending in the application.

    4a) Of the above claim(s) _____ is/are withdrawn from consideration.

5)☐ Claim(s) _____ is/are allowed.

6)☒ Claim(s) *1-69* is/are rejected.

7)☐ Claim(s) _____ is/are objected to.

8)☐ Claim(s) _____ are subject to restriction and/or election requirement.

Application Papers

9)☐ The specification is objected to by the Examiner.

10)☒ The drawing(s) filed on ~~15 February 2002~~ 5/2/02 is/are: a)☒ accepted or b)☐ objected to by the Examiner.

    Applicant may not request that any objection to the drawing(s) be held in abeyance. See 37 CFR 1.85(a).

11)☐ The proposed drawing correction filed on _____ is: a)☐ approved b)☐ disapproved by the Examiner.

    If approved, corrected drawings are required in reply to this Office action.

12)☐ The oath or declaration is objected to by the Examiner.

Priority under 35 U.S.C. §§ 119 and 120

13)☐ Acknowledgment is made of a claim for foreign priority under 35 U.S.C. § 119(a)-(d) or (f).

    a)☐ All b)☐ Some * c)☐ None of:

      1.☐ Certified copies of the priority documents have been received.

      2.☐ Certified copies of the priority documents have been received in Application No. _____ .

      3.☐ Copies of the certified copies of the priority documents have been received in this National Stage application from the International Bureau (PCT Rule 17.2(a)).

    * See the attached detailed Office action for a list of the certified copies not received.

14)☐ Acknowledgment is made of a claim for domestic priority under 35 U.S.C. § 119(e) (to a provisional application).

    a) ☐ The translation of the foreign language provisional application has been received.

15)☐ Acknowledgment is made of a claim for domestic priority under 35 U.S.C. §§ 120 and/or 121.

Attachment(s)

1)☒ Notice of References Cited (PTO-892)

2)☐ Notice of Draftsperson's Patent Drawing Review (PTO-948)

3)☒ Information Disclosure Statement(s) (PTO-1449) Paper No(s) *5* .

4)☐ Interview Summary (PTO-413) Paper No(s). _____ .

5)☐ Notice of Informal Patent Application (PTO-152)

6)☐ Other: .

Detailed Action

Claims Rejection – 35 U.S.C. 103

1. The following is a quotation of 35 U.S.C. 103(a) which forms the basis for all obviousness rejections set forth in this Office action:

(a) A patent may not be obtained though the invention is not identically disclosed or described as set forth in section 102 of this title, if the differences between the subject matter sought to be patented and the prior art are such that the subject matter as a whole would have been obvious at the time the invention was made to a person having ordinary skill in the art to which the subject matter pertains. Patentability shall not be negatived by the manner in which the invention was made.

2. Claims 1-69 are rejected under 35 U.S.C. 103(a) as being unpatentable over U.S. Patent Pub. No. 2002/0059047 to Haaland, in view of Obremski, U.S. Patent No. 5,498,875, and in further view of Gupta, U.S. Patent No. 5,319,586.

Regarding Claims 1-30, Haaland (047) discloses a set of hybrid least squares multivariate spectral analysis methods in which spectral shapes of components or effects not present in the original calibration step are added in a following prediction or calibration step to improve the accuracy of the estimation of the amount of the original

components in the sampled mixture. The hybrid method herein means a combination

of an initial calibration step with subsequent analysis by an inverse multivariate

analysis method. A spectral shape herein means normally the spectral shape of

a non-calibrated chemical component in the sample mixture but can also mean the

spectral shapes of other sources of spectral variation, including temperature drift,

shifts between spectrometers, spectrometer drift, etc. The shape can be continuous,

discontinuous, or even discrete points illustrative of the particular effect. See Abstract

Haaland (047) also discloses that recent advances in classical least squares

(CLS) algorithms have improved the range of problems that can be addressed with the

new prediction-augmented classical least-squares (PACLS) methods, see pending

application Ser. No. 09/518,351. It would be desirable to achieve the best features of

CLS or the new PACLS algorithm, and inverse algorithms such as the PLS or principal

component regression (PCR) factor analysis PCR algorithms. The combination of

CLS or PACLS and PLS or PCR (or any inverse least squares based method) for

spectral analysis is the subject of this invention. By combining the explicit/implicit

(hard/soft) modeling of CLS and inverse methods (e.g., PLS or PCR), the best

features of each method can be realized in a single hybrid method of spectral analysis.

Although the discussion concentrates on a PLS application, the new hybrid method

can accommodate any appropriate inverse factor analysis method. The invention

also includes any multivariate calibration method that uses or contains an inverse

method and allows spectral shapes (continuous or discontinuous) to be added directly

to the method during calibration or prediction or both, such addition performed without

solely weighting by a covariance matrix. See Page 2, Paragraph [0020].

Haaland (047) still further teaches that any spectral preprocessing should be

applied to the original calibration spectra, the prediction spectra, and the spectral

shapes added in the PACLS method. Preprocessing steps include but are not limited

to baseline correction, pathlength scaling, smoothing, derivatives, normalization,

variance or auto scaling, and Fourier transforms, as recited in Claim 4. When

pathlength scaling is performed, pathlength adjustments are normally applied by

dividing the spectra by the pathlength to compensate for the intensity variations

expected for pathlength changes in the individual samples. However, this procedure

scales all components of the spectra equally. Not all sources of spectral variation

should have this pathlength correction applied to them. Examples of spectral variation

than should not be scaled include, but are not limited to, drift of the spectrometer,

spectrally active purge gas components, and spectral changes external to the sample.

In order to properly handle these different spectral components, the effect of

pathlength scaling can be removed from the appropriate components by scaling the

non-pathlength component concentrations in the CLS calibration by the inverse of the

pathlength. This procedure effectively removes the effect of inappropriate scaling of

the non-pathlength spectral components.

A method to select the eigenvectors to include in the PACLS prediction from any

of the analyses discussed above is based upon the use of the CLS calibration model

to perform a CLS prediction on the eigenvector spectral shapes. Since the

eigenvectors are orthogonal basis vectors, the errors from the eigenvectors are

independent. Thus, the total error variance of all the spectral shapes included in the

eigenvector decomposition is the sum of the error variances of the individual errors

from each eigenvector. Therefore, the eigenvectors can be selected from those that

represent the largest error sources in the standard CLS calibration (or PACLS

calibration if spectral shapes are included during the building of the calibration model

and additional shapes are to be included during true prediction or validation). See

Page 5, Paragraph [0042] and [0043].

Haaland (047) as applied above does not specifically disclose the use of target

factor analysis, as recited in Claim 1. However, Obremski (875) discloses that

spectroscopic measurements have some uncertainty. If the predominant

uncertainty is not in the in the spectroscopic data, then the inverse least squares

method is preferred. Otherwise, the classical least squares method is preferred. The

fewer matrix inversions required by the inverse least squares approach tend to

outweigh the potential benefits of a change in coordinates during the regression steps.

Inverse least squares is the preferred method because of greater resistance to

problems with near singular matrices. The problems of matrix singularity in multiple

linear regression determinations is reduced by using orthogonalization methods. This

is an eigenvector analysis by singular value decomposition, or factor analysis. An

orthogonal matrix is one where all the column vectors are mutually perpendicular.

Orthogonalization of a matrix prior to an inverse least squares method permits

inversion of the matrix without singularity problems. This technique is principal

component regression. This technique is also known as P-matrix method, target

transform factor analysis or <u>target factor analysis</u>.

Therefore it would have been obvious to one of ordinary skill in the art that

Haaland's (824) multivariate spectral analysis method can be modified to use target

factor analysis in accordance with Obremski (875), to reduce problems with matrix

singularity.

Haaland (047) in view of Obremski (875), as applied above does not specifically

disclose the use of Gramm-Scmidt orthoganalization, as recited in Claim 12. However,

Gupta (586) discloses that Mathematical operations, consistent with the Gramm-

Schmidt method of orthogonalization, can now be performed on these n-1 vectors.

The result is that they are rotated in hyperspace so that they are orthogonal to each

other and remain orthogonal to the solution vector. This operation describes the

direction of the solution vector. The intersection of this directional vector with the

plane originally subtracted from the other n-1 planes determines the unique solution.

See Column 9, line28-36.

Therefore it would have been obvious to one of ordinary skill in the art that the

multivariate spectral analysis method of Haaland (824) in view of Obremski (875) can

be modified to use the Gramm-Scmidt orthogonalization method in accordance with

Gupta(586), to further reduce problems with matrix singularity.

Regarding Claims 31-69, Haaland (047) further discloses that the hybrid methods

disclosed can be used for any quantitative spectral analysis independent of the type of

spectroscopy used. These methods can be used in any spectroscopy where the

spectral data are related to the parameters of interest. In addition to quantitation,

qualitative and classification analyses can be performed with the hybrid algorithms.

Types of spectroscopy where these methods might be used include, but are not

restricted to, 1) infrared, 2) near-infrared, 3) visible, 4) ultraviolet, 5) X-ray, 6)

gamma-ray, 7) Raman, 8) mass spectroscopy, 9) ion-mobility mass spectroscopy,

10) Auger, 11) fluorescence, 12) phosphorescence, 13) ESCA, 14) far-infrared,

15) microwave, 16) x-ray fluorescence, 17) NMR, 18) energy loss spectroscopy,

19) EDAX, 20) ESR, and 21) multi- and hyper-spectral imaging. These spectroscopic

methods can be used in absorption, transmission, reflection, or emission modes. In

addition, the hybrid methods can be applied to other forms of multivariate data such as

seismic data, chromatographic data, thermal gravimetric analysis, and image data.

The hybrid algorithm can also be used for outlier or anomaly detection by examining

various outlier metrics such as Mahalanobis distance, spectral residuals, spectral F

ratios, or other statistical indications of spectra that lie outside the hybrid model. This

additional capability is ideally suited for multi- and hyperspectral image analysis. With

the outlier metrics obtained from hybrid algorithm, the hybrid method can also be used

for classification purposes. In this discussion, spectral components can include either

chemical components (molecular or elemental) <u>or other sources of spectral change

that include but are not limited to spectrometer/system drift</u>, chromatic aberrations,

diffraction effects, temperature changes, sample insertion and alignment effects, purge
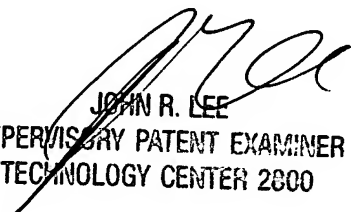
changes, alignment changes, detector changes and nonlinearities, source changes, and changes in spectrometer components to include even substitution of whole spectrometers. See Page 5, Paragraph[0027].

Conclusion

3. Any inquiry concerning this communication or earlier communications should be directed to Phillip Johnston whose telephone number is (703) 305-7022. The examiner can normally be reached on Monday-Friday from 7:30 am to 4:00 pm. If attempts to reach the examiner by telephone are unsuccessful, the examiners supervisor John Lee can be reached at (703) 308-4116. The fax phone numbers are (703) 872-9318 for regular response activity, and (703) 872-9319 for after-final responses. In addition the customer service fax number is (703) 872- 9317.

Any inquiry of a general nature or relating to the status of this application or proceeding should be directed to the receptionist whose telephone number is 703 308 0956.

PJ
May 16, 2003

JOHN R. LEE
SUPERVISORY PATENT EXAMINER
TECHNOLOGY CENTER 2800